

Application of Pareto Local Search and Multi-Objective Ant Colony Algorithms to the Optimization of Co-Rotating Twin Screw Extruders

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1 Introduction

Co-rotating twin screw extruders are extensively used in the polymer compounding industry mainly due to their good mixing capacity. Given its modular construction, this type of machines can easily be adapted to work with different polymeric systems, e.g., polymer blends, nanocomposites or highly filled polymers. Nevertheless, the performance of these machines is strongly dependent on the screw configuration and geometry. As a result, the definition of a best screw geometry to use in a specific polymer system is an optimization problem that involves selecting the location of a set of available screw elements along the screw axis. This optimization problem is a sequencing problem, where a permutation of a specific number of different screw elements must be determined. The sequence determines the position of screw elements along the screw axis, aiming at maximization performance. An additional complicating factor is the definition of the best screw configuration to use in a specific compounding/reactive extrusion operation. It involves several, often conflicting, objectives and, thus, it is a multi-objective combinatorial optimization problem (MCOP).

In previous work, a Multi-Objective Evolutionary Algorithm (MOEA) has been used to determine the best sequence of a pre-defined number of screw elements in co-rotating twin screw extruders [1]. In this work, we develop alternative algorithms for tackling this problem. In particular, we develop effective Stochastic Local Search (SLS) algorithms following the Pareto local search and two-phase local search frameworks [2, 3] as well as a Multi-Objective Ant Colony (MO-ACO) algorithm. We have carried out a detailed investigation of the sensitivity of the algorithms performance to changes of their parameters and a comparison to the previously designed MOEA using different objectives. This paper is organized as follows. The twin-screw extrusion configuration problem is described in section 2 and in section 3 we give details of the algorithms we use. Some experimental results with these algorithms are presented in section 4 and we conclude in section 5.

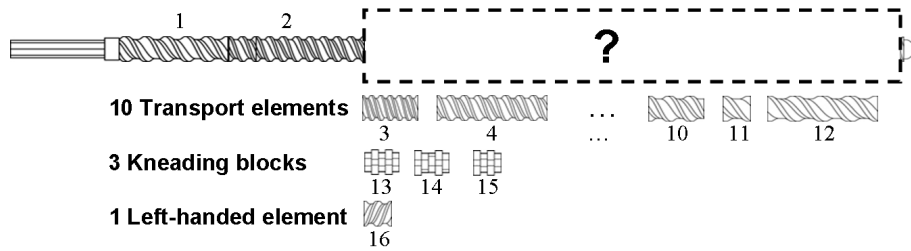


Figure 1: Twin-screw extrusion configuration problem

2 Twin-screw Extrusion Configuration Problem

The choice of an optimization methodology depends mainly on the type of problem to solve. We consider the case, where the problem of determining the best screw configuration consists in finding a sequence of a fixed number of screw elements of a twin screw extruder. This problem is illustrated in Figure 1; it involves the determination of the position along the screw of 10 transport elements, 3 kneading blocks (with different staggering angles) and one reverse element.

The flow behavior is induced by the different screw elements in dependence of their geometrical characteristics. Right handed elements have conveying properties while left handed and kneading blocks with a negative staggering angle induce restriction (generating pressure) to the flow. These are called restrictive elements. After the solid polymer is fed into a hopper, it will flow under starved conditions through transport elements. When a restrictive element is reached, the channel starts to fill up and the melting process takes place. When all polymer is melted, the flow occurs with or without pressure in the rest of the screw elements, depending on whether it is totally or partially filled; overall, pressure is determined by the location of the restrictive elements. The evaluation of the performance of each screw configuration is made by an elaborated computer simulation of the polymer flow through the screw elements that takes into account the relevant physical phenomena. Each evaluation of a screw configuration takes about one to two minutes on current CPUs. Hence, the high computational effort required for these evaluations is an additional complicating factor and we require algorithms that use a low number of function evaluations. In this example we consider the optimization goals average strain, specific mechanical energy (SME) and viscous dissipation. This problem we denote as Twin Screw Configuration Problem (TSCP).

3 Multi-Objective Optimization

3.1 Iterative improvement algorithms

SLS algorithms [5] have been successfully applied to single objective problems and, more recently also to MCOPs. Successful single-objective based SLS algorithms can be straightforwardly extended in two principled ways to multi-objective optimization problems [2, 3]. One possibility is to apply single-objective SLS algorithms to aggregations of the various objective functions into a single one. An alternative is to adopt a component-wise acceptance model, where a new solution is accepted if it is non-dominated. In this work, both strategies were tested using as underlying SLS methods iterative improvement algorithms. We use Pareto Local Search (PLS) as an example using a component-wise ordering search model [2], and the Two-Phase Local Search (TPLS), based on the scalarized acceptance criterion search model [3]. In both cases, the 2-swap operator was used to define the neighborhood relation: two solutions are considered to be neighbors if one can be obtained from the other by swapping the position of two screw elements [5].

Pareto Local Search The main ideas of PLS are the use of an archive, where all non-dominated solutions found so far are kept, and the exploration of the neighborhood of each of these solutions based on non-dominance criteria [2]. The algorithm starts with a random initial solution. This solution is added to the archive and its neighborhood is explored using the 2-swap operator. All non-dominated solutions identified in the neighborhood exploration are added to the archive, if they are not dominated by any of the solutions in the archive. If any solution in the archive would become dominated in this process, it is eliminated. These steps of solution selection and archive update are iterated until the neighbourhood of all solutions in the archive has been explored. In order to avoid a too strong increase of the number of solutions in the archive, an archive bounding technique was used [6]. This bounding technique divides the objective space by a grid into hypercubes and allows only one non-dominated solution to occupy a given hypercube.

Two-Phase Local Search In the TPLS algorithm, the various objectives are aggregated using a weighted sum and the search proceeds by occasional changes of the weights during successive steps [3]. The algorithm starts from a random initial solution optimising one specific objective (i.e., all weights are equal to zero except one). This solution is added to the archive being considered as the initial solution for the next search step. Then, a different set of weights is considered and the local search algorithm, starting from the solution returned for the previous weight vector, is applied until a new solution is found, which is added to the archive. The search process stops when all weight vectors are explored. As in [3], we follow a strategy that minimally changes the component-wise differences between the weight vectors. All non-dominated solutions found during this search process are added to the archive.

3.2 Multi-Objective Ant Colony Optimization

Ant Colony Optimization is a population-based algorithm that takes inspiration of real ants foraging behavior [4]. In recent years, several approaches have been proposed to apply this algorithm to multi-criteria optimization problems [7]. The ACO algorithm is based on a probabilistic solution construction, where the probabilities are a function of the pheromone strenghts on the ants' "trail". The solution components of the better or the best solutions receive reinforcement through the deposition of an amount of pheromone that typically depends on the solutions' quality. Simultaneously, the pheromone trails of all solution components are decreased by a pheromone evaporation mechanism. This process induces a search around the best solutions found.

ACO algorithms can be applied to multi-objective problems, for example, by changing the way the pheromone information is considered. Two different approaches are usually followed. The first approach consists in using a single pheromone matrix for all the objectives, while in the second approach one matrix for each objective is used [7]. When using a single pheromone matrix the solution construction follows the usual steps of the ACO algorithm. However, if for each objective one pheromone matrix is used, then the various pheromone informations are typically aggregated by using a weighted sum between the two pheromone matrices. In this case, for a specific ant m a screw element j will be chosen after a screw element i with a probability equal to:¹

$$p_{ij}^m = \frac{\tau_{ij}^{\lambda_1} \cdot \tau'_{ij}{}^{\lambda_2}}{\sum_{l \in N_i^l} \left[\tau_{il}^{\lambda_1} \cdot \tau'_{il}{}^{\lambda_2} \right]} \quad \text{if } j \in N_i^m$$

where N_i^m is the feasible neighborhood of the ant m (i.e., the screw elements which are still available) and λ_1, λ_2 with $\lambda_1 + \lambda_2 = 1$, are the weights given to each pheromone matrix. The exploration of different regions of the search space is accomplished by attributing different sets of weights to the

¹A pheromone model, where τ_{ij} refers to the desirability of assigning a screw element i to a position j in the sequence was also tested. However, this pheromone model was found to be inferior to the successor based one described above.

Screw	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Length	97.5	120	45	60	30	30	30	60	30	120	30	120	37.5	60	60	30
Pitch	45	30	KB-45	30	-20	60	30	20	KB-60	30	30	60	KB-30	45	30	20

Table 1: Configuration of the individual screw elements

Case Study	Objectives	Aim	X_{min}	X_{max}
1	Average Strain	Maximization	1000	15000
	Specific Mechanical Energy (SME)	Minimization	0.5	2
2	Average Strain	Maximization	1000	15000
	Viscous dissipation	Minimization	0.9	1.5
3	Specific Mechanical Energy (SME)	Minimization	0.5	2
	Viscous dissipation	Minimization	0.9	1.5

Table 2: Optimization objectives, aim of optimization and prescribed range of variation used in each case

different ants to be considered during the search process. All the non-dominated solutions generated along the successive iterations are stored in an archive. When one pheromone matrix for all objectives is applied, the update is done using a maximum of five non-dominated solutions that will deposit, each one, an amount of $1/k$, with k the number of ants allowed to update. On the other hand, if one matrix for each objective is applied only one ant is allowed to update each pheromone matrix choosing the one with the best respective objective function.

Two different strategies were tested in what concerns the pheromone update. One is based on the non-dominated solutions found in the current iteration (iteration-best strategy) and the other considers all the non-dominated solutions found so far (best-so-far strategy). The best strategy is the latter one and, for this reason, was adopted in the remaining of this work.

4 Results and Discussion

The performance of the algorithms presented above were tested using the individual screw elements presented on Table 1, for a Leistritz LSM 30-34 extruder, and the objectives presented on Table 2. Each optimization run was performed 10 times using different seed values. The comparison between the algorithms was made using the attainment functions methodology [8, 9].

4.1 MO-ACO results

To test the ability of the MO-ACO algorithm to deal with the TSCP problem, an initial study considering various values for the algorithm parameters (such as, pheromone evaporation, use of one or various pheromone matrices, different types of assignment of screw elements, use of the probability summation rule and use of various colonies) was performed. Figure 2 presents the results obtained for the Empirical Attainment Functions (EAFs) when comparing the use of one versus various (one for each objective) pheromone matrices for case study 1. The left of the figure represents the region of the Pareto frontier where the EAF obtained with one matrix is higher than the results obtained with various matrices, while on the right are represented the regions of the Pareto frontier where the second method is better. As can be seen, the performance when using various matrices is higher. Identical results were obtained for the remaining case studies.

Figure 3 represents three different screw configurations taken from the Pareto frontier shown. As expected, when the SME (objective to be minimized) increases, the restrictive elements are located downstream of the screw configuration (in case C the polymer will melt earlier because the restrictive elements are located earlier, and consequently, the energy necessary to rotate the screws is higher). The opposite is true when considering the Average Strain objective that is to be maximized.

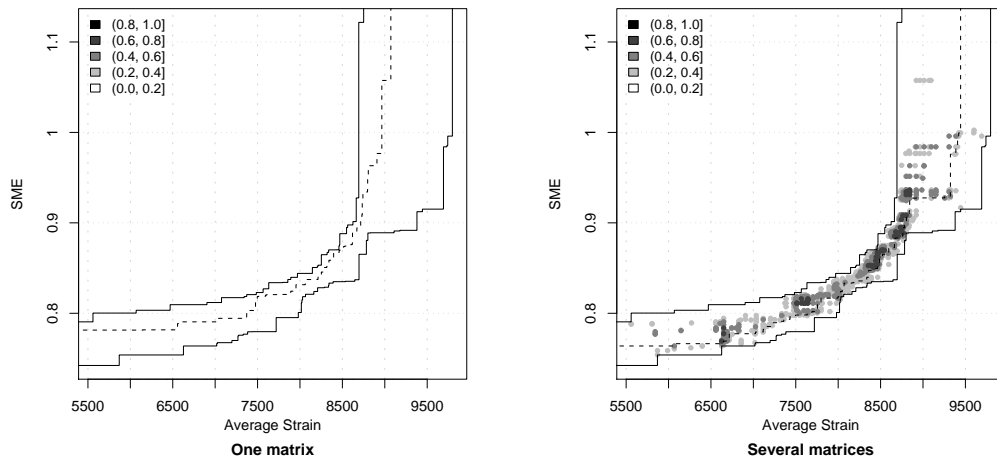


Figure 2: EAFs differences between the results obtained with MO-ACO using one or various pheromone matrices (case study 1)

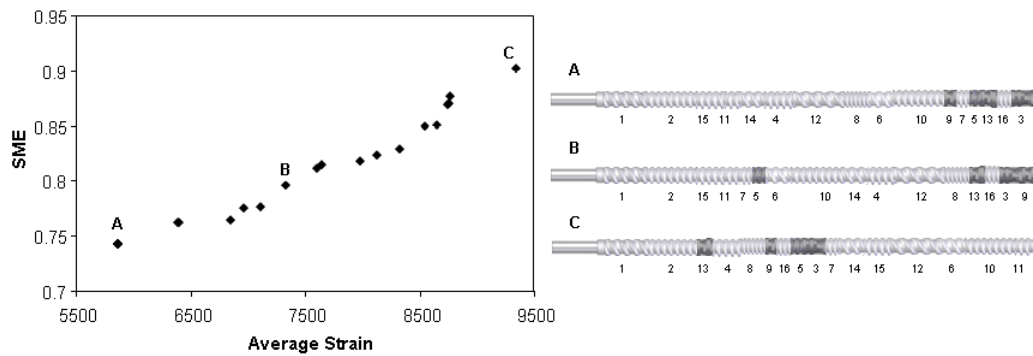


Figure 3: Pareto front for case study 1 and the screw configuration for solutions A to C

4.2 Comparison with SLS algorithms

Figure 4 shows an example of the comparison between MO-ACO and TPLS considering identical number of evaluations of the objective functions. Identical results are obtained for the remaining case studies. As can be seen, the TPLS algorithm appears to be significantly better than MO-ACO especially in the center of the fronts. In fact, further comparisons have shown that typically the SLS algorithms also improve upon the performance of the previously applied MOEA.

5 Conclusions

Simple SLS algorithms and MO-ACO algorithms have been applied with success to the Twin Screw Configuration Problem. The solutions obtained are in agreement with the knowledge about the process and have physical meaning. The good performance obtained with the simple SLS algorithms indicates that the development of a hybrid algorithm through the incorporation of iterative improvement methods

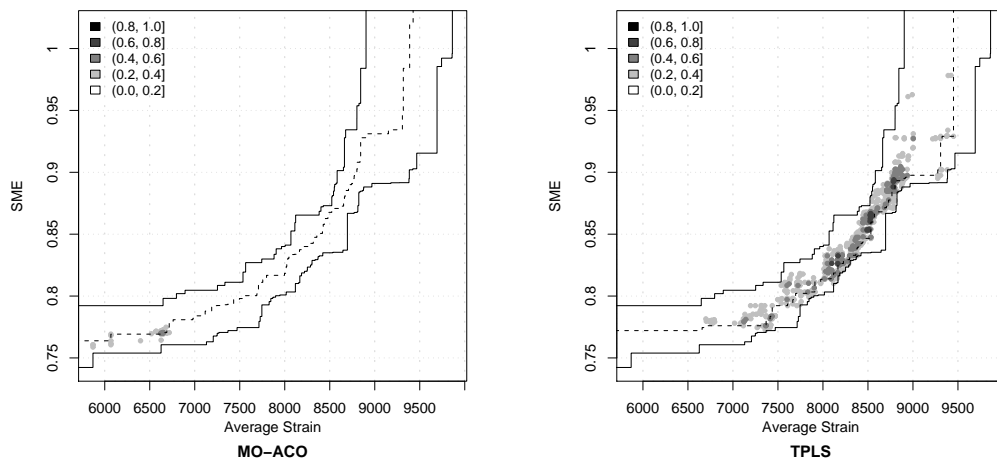


Figure 4: EAFs differences between the results obtained with MO-ACO and TPLS (case study 1)

into the MO-ACO algorithm can be a good way to further improve performance.

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